

10/576,703

of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 07:59:27 ON 09 MAY 2007

=> file casreact

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'CASREACT' ENTERED AT 07:59:36 ON 09 MAY 2007

USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT

COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications.

FILE CONTENT:1840 - 5 May 2007 VOL 146 ISS 20

New CAS Information Use Policies, enter HELP USAGETERMS for details.

*
* CASREACT now has more than 12 million reactions *
*

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>
Uploading C:\Program Files\Stnexp\Queries\10 series\10576703\1.str



chain nodes :

1 2 3 4 5 6 7 8 17 18 19 20 21 22 23 24 27 29 31

ring nodes :

9 10 11 12 13 14 15 16

chain bonds :

Compounds - May 8, 2007

10/576,703

1-2 2-3 2-4 4-5 5-6 6-7 6-8 10-17 12-19 14-18 16-20 21-22 21-27 21-29 23-24
29-31
ring bonds :
9-10 9-13 9-16 10-11 11-12 12-13 13-14 14-15 15-16
exact/norm bonds :
9-10 9-13 9-16 10-11 10-17 11-12 12-13 12-19 13-14 14-15 14-18 15-16 16-20
21-22 21-27 21-29 23-24 29-31
exact bonds :
2-4 4-5 5-6
normalized bonds :
1-2 2-3 6-7 6-8

G1:H,CH3,CF3,CN,X,[*1]

G2:C,S,N

G3:Cb,Ak

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS 19:Atom
20:Atom 21:Atom 22:CLASS 23:CLASS 24:CLASS 27:CLASS 29:CLASS 31:CLASS
fragments assigned product role:
containing 9
fragments assigned reactant/reagent role:
containing 1
containing 21

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full

FULL SEARCH INITIATED 07:59:57 FILE 'CASREACT'

SCREENING COMPLETE - 18 REACTIONS TO VERIFY FROM 2 DOCUMENTS

100.0% DONE 18 VERIFIED 0 HIT RXNS 0 DOCS

SEARCH TIME: 00.00.01

L2 0 SEA SSS FUL L1 (0 REACTIONS)

=>

Uploading C:\Program Files\Stnexp\Queries\10 series\10576703\2.str



chain nodes :

9 10 11 12 13 14 15 16 19 21 23

ring nodes :

1 2 3 4 5 6 7 8

chain bonds :

2-9 4-11 6-10 8-12 13-14 13-19 13-21 15-16 21-23

ring bonds :

1-2 1-5 1-8 2-3 3-4 4-5 5-6 6-7 7-8

exact/norm bonds :

1-2 1-5 1-8 2-3 2-9 3-4 4-5 4-11 5-6 6-7 6-10 7-8 8-12 13-14 13-19 13-21
15-16 21-23

G1:H,CH3,CF3,CN,X, [*1]

G2:C,S,N

G3:Cb,Ak

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:CLASS

11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS 19:CLASS 21:CLASS 23:CLASS

fragments assigned product role:

containing 1

fragments assigned reactant/reagent role:

containing 13

L3 STRUCTURE UPLOADED

=> d

L3 HAS NO ANSWERS

L3 STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

=> s 13 full

FULL SEARCH INITIATED 08:00:21 FILE 'CASREACT'

10/576,703

SCREENING COMPLETE - 2371 REACTIONS TO VERIFY FROM 244 DOCUMENTS
100.0% DONE 2371 VERIFIED 5 HIT RXNS 3 DOCS
SEARCH TIME: 00.00.03

L4 3 SEA SSS FUL L3 (5 REACTIONS)

=> d ibib hit 1-3